Three-fermion problems in optical lattices

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We present exact results for the spectra of three fermionic atoms in a single well of an optical lattice. For the three lowest hyperfine states of ^{6}Li atoms, we find a Borromean state across the region of the distinct pairwise Feshbach resonances. For ^{40}K atoms, nearby Feshbach resonances are known for two of the pairs, and a bound three-body state develops towards the positive scattering-length side. In addition, we study the sensitivity of our results to atomic details. The predicted few-body phenomena can be realized in optical lattices in the limit of low tunneling.

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Introduction.– Experiments with cold atomic gases make it possible to study strong-interaction physics in a controlled manner. When an atomic gas is loaded into an optical lattice, typically a few atoms reside in each well. Therefore, optical lattices can be used to investigate few-body phenomena when the tunneling barrier between potential wells is high [1]. In dilute gases, the interactions are governed by the S-wave scattering length a, which can be tuned across atomic Feshbach resonances. Consequently, three-fermion problems in optical lattices can access nearly the entire landscape of fascinating few-body phenomena. When all scattering lengths are large, the few-body physics of dilute gases exhibits universal properties because there are no length scales associated with the interaction. These universal aspects stretch across physics: For example, the large scattering-length physics predicts a linear correlation for ground-state energies of few-helium clusters or light nuclei [2].

The first step towards realizing isolated few-atom systems was the formation of molecules from fermionic atoms in an optical lattice [3]. In addition, the ground-state energy of two particles in a single well of an optical lattice was measured across a Feshbach resonance by rf dissociation to noninteracting fragments. The measured ground-state energies (for varying scattering length) agree very well with the theoretical prediction for two particles in a harmonic oscillator potential [3].

For three identical bosons, the scattering lengths of all pairs can be tuned with one Feshbach resonance and the three-boson problem is universal: On resonance, there is an infinite tower of Efimov trimer states with consecutive binding energies $E_n/E_{n+1} \approx 515$ in free space [4]. Efimov states become bound for a finite, negative scattering length, and lead to resonances in the rate for three-body recombination. Recently, the first Efimov resonance was observed in a gas of cold Cæsium bosons [5]. For three particles in a harmonic well, the spatial confinement restricts the size of the Efimov states, and thus the accumulation of bound states does not persist. However, Stoll and Köhler have shown that it is possible to study the first Efimov state isolated in a single well of an optical lattice [6]. This three-boson problem was also studied by Jonsell *et al.* in an adiabatic approximation [7]. Efimov trimers can be examples of Borromean systems (when the scattering length is negative): three-body bound states for which all pairs are unbound. Other Borromean systems are the ^{6}He nucleus and the ^{11}Li halo nucleus (^{4}He or ^{9}Li and two neutrons) [8].

For fermions, in contrast to identical bosons, the Pauli principle restricts S-wave interactions to different hyperfine states, which have distinct pairwise Feshbach resonances. In this Letter, we calculate exactly the spectra of the three lowest hyperfine states of ^{6}Li or ^{40}K atoms confined to a single harmonic well of an optical lattice, using effective field-theory interactions. For ^{6}Li atoms, there are Feshbach resonances between all pairs [9], two of which overlap closely, and we find a Borromean state that extends across all Feshbach resonances. For ^{40}K atoms, Feshbach resonances exist between two pairs, whereas the third pair interacts weakly. In this case, we find that a three-body state only develops towards the positive scattering-length side, and is bound around the doubly-interacting particle. The spectra for three ^{6}Li or ^{40}K atoms in optical lattices are very rich, and the Bloch-Horowitz method employed here is ideally suited to identify the angular momenta of the states. The predicted few-body phenomena can be realized in optical lattices in the limit of low tunneling.

Three-fermion problems.– Across a Feshbach resonance the dependence of the scattering length on the magnetic field B is given by $a(B) = a_{\rm bg}(1 - \Delta/[B - \overline{B}])$ where $\overline{B}$ and Δ are the position and width of the resonance and $a_{\rm bg}$ denotes the background scattering length. For ^{6}Li, the three trapped hyperfine states are the lowest magnetic sub-states: $|1\rangle = |F, m_F\rangle = |1/2, 1/2\rangle$, $|2\rangle = |1/2, -1/2\rangle$ and $|3\rangle = |3/2, -3/2\rangle$, with distinct Feshbach resonances, as shown in Fig. 1. The resonance positions are $\overline{B}_{12} = 83.41\,\mathrm{mT}$, $\overline{B}_{13} = 69.04\,\mathrm{mT}$ and $\overline{B}_{23} = 81.12\,\mathrm{mT}$ [9], and we use the Feshbach parameters plus leading-order correction determined in [9]. The relevant hyperfine states for ^{40}K are $|1\rangle = |F, m_F\rangle = |9/2, -9/2\rangle$, $|2\rangle = |9/2, -7/2\rangle$ and $|3\rangle = |9/2, -5/2\rangle$.

As shown in Fig. 2, nearby Feshbach resonances are present between the states 12 and 13, with Feshbach parameters: $\overline{B}_{12} = 202.10\,\mathrm{G}$ [10], $\Delta_{12} = 7.8\,\mathrm{G}$ [12], $\overline{B}_{13} = 224.21\,\mathrm{G}$, $\Delta_{13} = 9.7\,\mathrm{G}$ [11] and background scattering length $a_{\mathrm{bg}} \approx 174\,a_0$ [11].

We work with effective field-theory contact interactions regulated by separable cutoff functions [13]

$$V(p', p) = \frac{4\pi\hbar^2}{m}\, g(B,\Lambda)\, e^{-(p'^2+p^2)/\Lambda^2}\,, \qquad (1)$$

where p and p' denote incoming and outgoing relative momenta, and the coupling $g(B,\Lambda)$ is determined from the scattering length through $g(B,\Lambda) = a(B)/(1 - \Lambda a(B)/\sqrt{2\pi})$. If a is weak ($a \sim R$, where R is the range of the interaction), it is possible to choose the cutoff in a wide range with $|\Lambda a| \ll 1$, and one recovers the standard pseudo-potential for low momenta $V(0,0) = 4\pi\hbar^2 a/m$. The cutoff generates an effective range $r_{\mathrm{e}} \sim 1/\Lambda$ and higher-order terms, which we render small with large cutoffs. In addition we can vary Λ. This probes neglected effective range effects and sensitivity to atomic details.

For the separable interaction, Eq. (1), the two-body problem in a harmonic oscillator potential can be solved exactly. Following Busch *et al.* [14], the intrinsic energy $E = \epsilon\,\hbar\omega$ is given by

$$\frac{{}_2F_1\left(\frac{3}{2}, \frac{3}{4} - \frac{\epsilon}{2}; \frac{7}{4} - \frac{\epsilon}{2}; \left[\frac{1-x^2}{1+x^2}\right]^2\right)}{\left(1 + \frac{1}{x^2}\right)^3 \left(\frac{\epsilon}{2} - \frac{3}{4}\right)} + x = \frac{\sqrt{2\pi}}{a/b}\,, \qquad (2)$$

where ${}_2F_1$ is the hypergeometric function, $x = \Lambda b$ and $b = \sqrt{\hbar/m\omega}$ is the oscillator length. For large cutoffs $x \to \infty$, we recover the result of Busch *et al.*, $\sqrt{2}\,\Gamma(\frac{3}{4} - \frac{\epsilon}{2})/\Gamma(\frac{1}{4} - \frac{\epsilon}{2}) = b/a$ [14]. The energy from Eq. (2) is within 3% (or 7%) of the latter for $\Lambda b = 100$ and all scattering lengths except the tight-binding region $0 < a/b \leqslant 1$ (or 0.5). Typical well frequencies in optical lattices are $\nu \sim 100\,\mathrm{kHz}$. Consequently, the oscillator length $b \sim 1000\,a_0$ (a_0 denotes the Bohr radius) is large compared to the range of atomic interactions $R \sim 10\,a_0$. Finally, the measured ground-state energies of two particles in a single well of an optical lattice agree very well with this result [3] even down to $|a/b| \approx 1$.

Bloch-Horowitz method.– The spectrum for the intrinsic energy of three hyperfine states in a harmonic well is determined from the three-body Hamiltonian

$$H = H_0 + V = \sum_{i=1}^{3} H_0(\mathbf{r}_i) - H_{0,\mathrm{cm}}(\mathbf{R}) + V_{12}(\mathbf{r}_1, \mathbf{r}_2) + V_{13}(\mathbf{r}_1, \mathbf{r}_3) + V_{23}(\mathbf{r}_2, \mathbf{r}_3)\,, \qquad (3)$$

where the noninteracting part is given by $H_0(\mathbf{r}) = -\hbar^2\nabla_{\mathbf{r}}^2/2m + m\omega^2 r^2/2$ and $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3)/3$ denotes the center-of-mass (cm) coordinate ($H_{0,\mathrm{cm}}$ uses mass $3m$). Within Jacobi coordinates, the eigenstates of H_0 are characterized by

$$H_0\,|12, 3\rangle = (N+3)\,\hbar\omega\,|12, 3\rangle\,. \qquad (4)$$

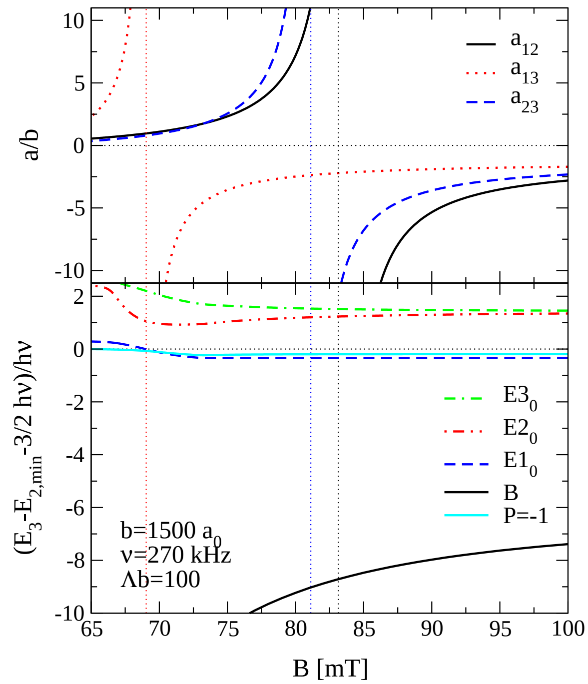

FIG. 1: Top: Feshbach resonances between the three lowest hyperfine states of ^{6}Li atoms [9]. Bottom: The spectrum for the above ^{6}Li states in a single well of an optical lattice with $\nu = 270\,\mathrm{kHz}$ versus magnetic field. These BH results are for $\Lambda b = 100$. The three-body energy E_3 is measured from the three-body dissociation threshold given by the minimal two-body energy $E_{2,\mathrm{min}}$ (from Eq. (2)) of the pairs and the additional particle in the noninteracting ground state $E_1 = 3/2\hbar\omega$ ($5/2\hbar\omega$ for the negative parity state P=-1). For $B >(<) 73.2\,\mathrm{mT}$, $E_{2,\mathrm{min}}$ is determined from $a_{12}(a_{23})$. The state labeled B is the Borromean state, and En_L denotes the n-th excited state with angular momentum L.

Here, $12 \equiv n_{12}, l_{12}, m_{12}$ are the radial, angular and magnetic quantum numbers of the pair 12, and $3 \equiv n_3, l_3, m_3$ refer to the quantum numbers of the third particle with respect to the cm of pair 12. We classify these noninteracting states $|N_i\rangle$ according to their principal quantum number $N = 2n_{12} + l_{12} + 2n_3 + l_3$, where the subindex i denotes all possible states for fixed total N.

We solve the three-body problem $(H_0 + V)|\psi(E)\rangle = E|\psi(E)\rangle$ using the Bloch-Horowitz (BH) approach [15, 16]. The BH method diagonalizes an effective Hamiltonian in a truncated space of $P = \sum_{N_i \leqslant N_{\max}} |N_i\rangle\langle N_i|$ low-energy excitations, such that the low-lying spectrum is exactly reproduced. Inserting $1 = P + Q$, we obtain the projections of the three-body Schrödinger equation:

$$P(H_0 + V)(P + Q)|\psi(E)\rangle = E\,P|\psi(E)\rangle\,, \qquad (5)$$

$$Q(H_0 + V)(P + Q)|\psi(E)\rangle = E\,Q|\psi(E)\rangle\,. \qquad (6)$$

Since $[P, H_0] = [Q, H_0] = 0$ and $PQ = 0$, we can solve Eq. (6) for $Q|\psi(E)\rangle = (E - H_0)^{-1}QV|\psi(E)\rangle$ and insert the latter into Eq. (5). This leads to the equivalent prob-

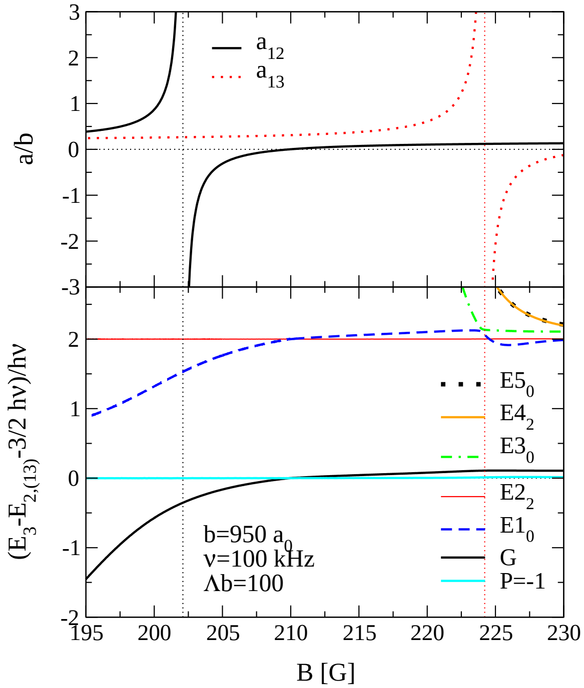

FIG. 2: Top: Feshbach resonances between the three lowest hyperfine states of ^{40}K atoms [10-12]. Bottom: The spectrum for the above ^{40}K states in a single well of an optical lattice with $\nu = 100\,\mathrm{kHz}$ versus magnetic field. These BH results are for $a_{23} = 0$ and $\Lambda b = 100$. The three-body energy E_3 is measured from the three-body dissociation threshold given by the ground-state energy of pair 13 ($E_{2,(13)}$) and the additional particle in $E_1 = 3/2\hbar\omega$ ($5/2\hbar\omega$ for P=-1). The state labeled G is the three-body ground state and En$_L$ is as in Fig. 1.

lem in the truncated space,

$$P\left(H_0 + V + V\frac{Q}{E - H_0}V\right)P|\psi(E)\rangle = E\,P|\psi(E)\rangle\,, \quad (7)$$

where the effective Hamiltonian $H_{\text{eff}}(E)$ (given by the operator in parentheses in Eq. (7)) depends self-consistently on the exact energy and exactly reproduces the low-lying spectrum, as long as the eigenstate has overlap with the truncated space $P|\psi(E)\rangle \neq 0$. Finally, we use a Faddeev decomposition $|\psi(E)\rangle = (1 + P_{12}P_{13} + P_{12}P_{23})|\psi(E)\rangle_{12}$ to construct $H_{\text{eff}}(E)$ (P_{ij} is the permutation operator).

The good quantum numbers of the interacting eigenstates are parity P, total angular momentum L and projection L_z: $|\psi(E)\rangle = |E; P, L, L_z\rangle$. Here we solve the BH Eq. (7) in an uncoupled basis for $L_z = 0$ ($m_{12} = m_3 = 0$). Since $|E; P, L_z\rangle = \sum_L C_L(E; P, L_z)\,|E; P, L, L_z\rangle$, the resulting spectra automatically contain states with all possible angular momentum quantum numbers. We will use the BH overlap condition to identify their angular momenta. The BH method has been used to calculate the ground-state properties of light nuclei [16], and as a check, we have reproduced the results of Stoll and Köhler for three identical bosons [6]. For the separable interaction, Eq. (1), it is possible to calculate the necessary BH two-body matrix elements analytically. In addition, we have found it sufficient to keep $l_{12}, l_3 \leqslant 3$.

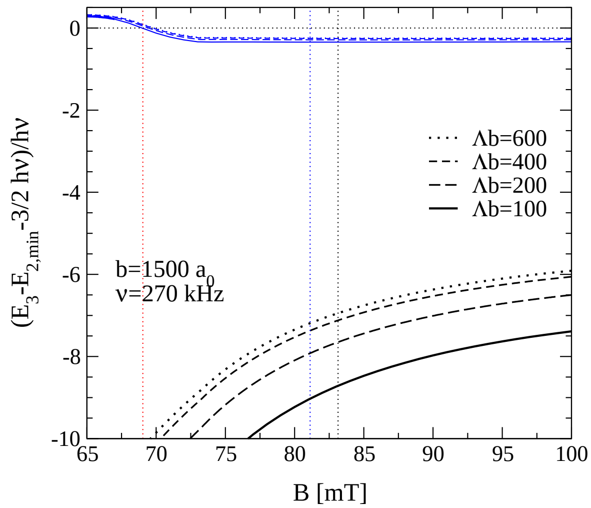

FIG. 3: The cutoff dependence of the Borromean and the first excited state of three ^{6}Li atoms versus magnetic field.

Results.– The magnetic field dependence of the spectrum for three ^{6}Li atoms in an optical lattice with $\nu = 270\,\mathrm{kHz}$ is shown in Fig. 1. The BH results are independent of $N_{\max}$. In particular, all states are present in the lowest $N_{\max} = 0$ calculation (with $l_{12} = l_3 = 0$), and thus all positive parity states shown have angular momentum $L = 0$. The lowest negative parity state has $L = 1$.

We find a deeply-bound Borromean state B that exists on the negative scattering length side and extends across the Feshbach resonances. Note that there are many very deeply-bound two-body states present. This state can be viewed as a collective state within a schematic model [17]. For $B > 75\,\mathrm{mT}$, the excited and negative parity states depend very weakly on the magnetic field in Fig. 1, since the Feshbach resonances of a_{12} and a_{23} are very close and here this two-body energy is subtracted. The first excited state E1$_0$ is adiabatically connected to the noninteracting $N = 0$ state at high magnetic fields. Similarly, the states E2$_0$ and E3$_0$ connect to the two $N = 2$ states with $l_{12} = l_3 = 0$, where the other three states of the noninteracting $N = 2$, $L_z = 0$ multiplet are higher in energy since they are less sensitive to S-wave interactions.

In Fig. 2 we show the spectrum for three ^{40}K atoms in an optical lattice with $\nu = 100\,\mathrm{kHz}$ versus magnetic field. In this case, there are two Feshbach resonances between pairs 12 and 13, and we have taken the third pair to be noninteracting $a_{23} = 0$ in this calculation. We find that a bound three-body state only develops towards the positive scattering-length side of both resonances. The three-body state is bound by the doubly-interacting particle 1. The qualitative features of the spectrum do not depend on a_{23} for $|a_{23}/a_0| \lesssim 100$. For instance, with a

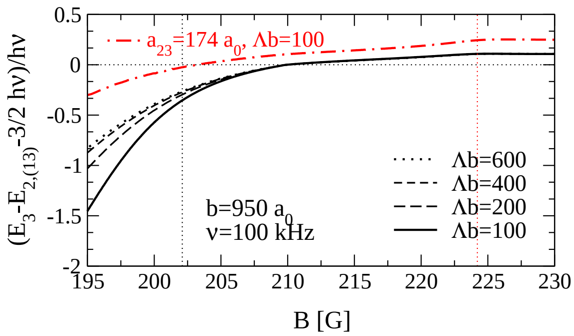

FIG. 4: The cutoff dependence of the ground state of three ^{40}K atoms versus magnetic field.

repulsive $a_{23} = a_{\rm bg} \approx 174\,a_0$, the spectrum is moved up and the ground state becomes bound only for lower magnetic fields (see Fig. 4, note that the precise value of a_{23} has not been calculated).

Two of the states of Fig. 2 ($E2_2$ and $E4_2$) are not present in a $N_{\rm max} = 0$ calculation, but exist for all larger $N_{\rm max} \geqslant 2$, and thus have angular momentum $L = 2$. At high magnetic fields, we recover the five states adiabatically connected to $N = 2$ (note $l_{13} = l_2 = 1$ can couple to $L = 0$, and also the avoided level crossing for two of the $L = 0$ states). For $B_0 = 209.9\,$G, we have $a_{12}(B_0) = 0$, and the only interaction is for pair 13. Therefore, the low-lying states are $E_3 - E_{2,(13)} - 3/2\hbar\omega = 2n_2 + l_2$ for the positive parity state (the excitation of the cluster 13 comes higher in energy; and $2n_2 + l_2 - 1$ with $-5/2\hbar\omega$ for P=-1), in agreement with Fig. 2. The states $E2_2$ ($l_2 = 2$) and P=-1 ($l_2 = 1$) follow only the two-body energy of the right Feshbach resonance. Finally for $B > B_0$, the interaction between 12 becomes weakly repulsive, which requires $\Lambda_{12} a < \sqrt{2\pi}$. Our ^{40}K results are for $\Lambda b = 100$, except $\Lambda_{12} a_{\rm bg} = 1$ for $B > B_0$. For $\Lambda_{12} a < \sqrt{2\pi}$, we find a very weak cutoff dependence from the repulsive part of the 12 interaction.

We can vary the cutoff and thus probe the dependence of our results to the effects of an effective range and many-body interactions [13]. In Figs. 3 and 4, we show the cutoff dependence of the Borromean and first excited states for ^{6}Li, and the ground state of the ^{40}K three-body problem. While this excited state (and all others) are well converged, the ground state energies converge slower and show a sizeable dependence on Λb, as the binding energy increases. Therefore, these states become sensitive to further atomic details, such as the effective range. Our results also indicate that there is no limit cycle in a harmonic oscillator potential with $b/R \lesssim 100$, and thus the power-counting of three-body interactions in the corresponding effective field theory (EFT) must change compared to free space. This may be important for a pionless EFT [13] for nuclei in an oscillator basis.

Conclusions.– Optical lattices open a frontier to controlled strong-interaction few-body physics, in addition to simulating condensed matter models. In this Letter, we investigated three-fermion problems in optical lattices for ^{6}Li and ^{40}K atoms using the BH method. For ^{6}Li atoms, we find a Borromean state on the negative scattering-length side that extends across the Feshbach resonances. In contrast, for ^{40}K atoms, one of the pairs interacts non-resonantly at the relevant magnetic fields, and a three-body state, bound by the doubly-interacting particle, develops towards the positive scattering-length side. While the quantitative results of the ground states are somewhat sensitive to atomic details, these features are independent thereof and also independent of the precise oscillator frequency. The three-fermion spectra are very rich, and we have identified the nature and angular momenta of all low-lying states. We predict a Borromean state in optical lattices under the conditions of overlapping or close Feshbach resonances for all pairs and attractive background scattering lengths.

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[1] D. Jaksch, *et al.*, Phys. Rev. Lett. **89**, 040402 (2002).
[2] E. Braaten and H.-W. Hammer, Phys. Rep. **428**, 259 (2006).
[3] T. Stöferle, *et al.*, Phys. Rev. Lett. **96**, 030401 (2006).
[4] V.N. Efimov, Phys. Lett. **33B**, 563 (1970); V.N. Efimov, Sov. J. Nucl. Phys. **12**, 589 (1971).
[5] T. Kraemer, *et al.*, Nature **440**, 315 (2006).
[6] M. Stoll and T. Köhler, Phys. Rev. **A72**, 022714 (2005).
[7] S. Jonsell, H. Heiselberg and C.J. Pethick, Phys. Rev. Lett. **89**, 250401 (2002).
[8] M.V. Zhukov, *et al.*, Phys. Rep. **231**, 151 (1991).
[9] M. Bartenstein, *et al.*, Phys. Rev. Lett. **94**, 103201 (2005).
[10] C.A. Regal, M. Greiner and D.S. Jin, Phys. Rev. Lett. **92**, 040403 (2004); Phys. Rev. Lett. **92**, 083201 (2004).
[11] C.A. Regal and D.S. Jin, Phys. Rev. Lett. **90**, 230404 (2003).
[12] C.A. Regal, *et al.*, Phys. Rev. Lett. **90**, 053201 (2003).
[13] P.F. Bedaque and U. van Kolck, Ann. Rev. Nucl. Part. Sci. **52** (2002) 339.
[14] T. Busch, *et al.*, Found. Phys. **28**, 549 (1998).
[15] C. Bloch and J. Horowitz, Nucl. Phys. **8**, 91 (1958).
[16] W.C. Haxton and C.-L. Song, Phys. Rev. Lett. **84**, 5484 (2000); W.C. Haxton and T. Luu, Phys. Rev. Lett. **89**, 182503 (2002).
[17] G.E. Brown and M. Bolsterli, Phys. Rev. Lett. **3**, 472 (1959).